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Integrated techno-economic and environmental analysis of butadiene production from biomass

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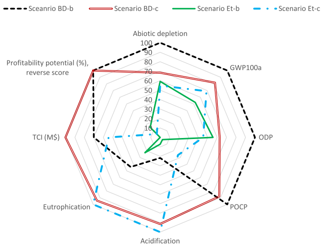
HIGHLIGHTS

- Techno-economic and environmental study of butadiene process annexed to sugar mill.
- Fossil-based butadiene (BD) and bioethanol production considered as the baseline.
- Co-combustion of coal with biomass improves the economic due to economies of scale.
- Bio-BD shows better performance over the investigated environmental impact categories.
- Bioethanol production has higher probability of economic feasibility than Bio-BD.

GRAPHICAL ABSTRACT



BD: Butadiene; Et: Ethanol; -b: Energy self-sufficient; -c: Coal co-combustion

Economic and environmental comparison of investigated biorefinery scenarios

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ABSTRACT

In this study, lignocellulose biorefineries annexed to a typical sugar mill were investigated to produce either ethanol (EtOH) or 1,3-butadiene (BD), utilizing bagasse and trash as feedstock. Aspen simulation of the scenarios were developed and evaluated in terms of economic and environmental performance. The minimum selling prices (MSPs) for bio-based BD and EtOH production were 2.9–3.3 and 1.26–1.38-fold higher than market prices, respectively. Based on the sensitivity analysis results, capital investment, Internal Rate of Return and extension of annual operating time had the greatest impact on the MSP. Monte Carlo simulation demonstrated that EtOH and BD productions could be profitable if the average of ten-year historical price increases by 1.05 and 1.9-fold, respectively. The fossil-based route was found inferior to bio-based pathway across all investigated environmental impact categories, due to burdens associated with oil extraction.

1. Introduction

1,3-Butadiene (BD) is one of the major building blocks in production of synthetic rubbers and polymers (Ochoa et al., 2016), with a global demand of 10 million tonnes in 2012 (Makshina et al., 2014) and rapid production growth specifically in Asia (Cespi et al., 2016; Sushkevich et al., 2015). Polybutadiene (PBR) and styrene-butadiene rubber (SBR) are the main end uses for BD including 54% of total usage in 2014. About 70% of PBR and one-third of SBR are utilized for tires. Therefore at least one-third of all BD produced eventually ends up in tires (Loh, 2015). Nowadays, the dominant technology for production of butadiene is thermal cracking, while catalytic and oxidative dehydrogenation of n-butane is also used on industrial scale (White, 2007). However, lower costs and larger availability of ethane from natural gas or shale gas resulted in replacement of naphtha with ethane as the

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feedstock in the cracking process after 1970s, which has lower BD yield. Consequently, restriction on the available BD in the market and price increase in the near future is expected (Cespi et al., 2016). Nevertheless, naphtha still represents the primary material for BD production (55%), followed by ethane (30%) (Cespi et al., 2016). An alternative approach is production of BD from ethanol, following one-stage (Lebedev) process commercialised in Russia during 1920s (Lebedev, 1933) or two-stage (Ostromisslensky) process, which was commercialised in USA by the Carbon and Carbide chemical corporation (Toussaint et al., 1947). However, after 1960s as a consequence of the lower price of oil, both ethanol-based processes became economically unfavourable and were stopped (Sushkevich et al., 2015). The ethanol route only survived in China and India up to now (Makshina et al., 2014).

Overall, thermal cracking of naphtha contribute strongly to environmental burdens, due to high emission of CO_2 and is considered as an energy intensive process (Ren et al., 2006). Considering recent social, political and economic interests in utilization of renewable and sustainable resource of energy, chemicals and materials, as well as more than 3.5 million tonnes synthetic rubber produced from BD annually, development of an alternative, sustainable process for BD production would create a very positive impact in the rubber industry (Isikgor and Becer, 2015). In fact, the three largest tyre manufacturers (Goodyear, Michelin, and Bridgestone) are working to develop the production of renewable rubber monomers from biomass resources (Isikgor and Becer, 2015). Also, Axens, IFPEN and Michelin have launched a joint research program in 2013 to develop a feasible process for production of synthetic rubber from bioethanol (Makshina et al., 2014). In addition, exploitation of bioethanol as a feedstock to build chemicals, rather than its utilisation as a fuel, seems more economical, while retaining possible benefits of greenhouse gas (GHG) emission reductions (Hanif et al., 2017).

Previous research studies on bio-based butadiene production have mostly focused on the reaction pathways and kinetics of ethanol to BD conversion, which are complicated (Makshina et al., 2012). However, it is generally accepted that ethanol is first dehydrogenated to acetaldehyde, followed by reaction between ethanol and acetaldehyde to produce BD. The yield and selectivity of BD production depends strongly on the choice of catalyst and reaction conditions. Different type of catalysts, i.e. single, binary and ternary metal oxides, have been evaluated for Lebedev (1-step) and Ostromisslensky (2-step) processes (Ochoa et al., 2016; Sushkevich et al., 2015). A comprehensive comparison of different catalysts evaluated for both ethanol routes is presented by Makshina et al., based on BD yield and selectivity (Makshina et al., 2014). Though many studies have focused on catalyst preparation and evaluation, only a few instances investigated economic or environmental evaluation of BD production, based only on the 1G pathway for ethanol production (Cespi et al., 2016).

However, the success of ethanol-based BD production depends on catalyst cost and performance, as well as the cost of up-stream bio-ethanol production and feedstock. Lignocellulosic ethanol production is the most studied second generation (2G) biorefinery, which has been investigated considering different process options (Haghighi Mood et al., 2013), feedstock types (De Laporte et al., 2016; Kurian et al., 2013), techno-economic evaluations (Quintero et al., 2013), supply chain modelling (De Laporte et al., 2016; Osmani and Zhang, 2014) and life cycle assessments (Osmani and Zhang, 2014). Several commercial 2G ethanol production plants are located in the USA (Peplow, 2014), Brazil (Chum et al., 2014) and the EU (Balan et al., 2013), with continuing technology development (Karimi and Chisti, 2015). Among the studied 2G feedstocks, sugarcane residues (bagasse and trash) is a high volume agriculture residue with global production estimated at approx. 810 million tonnes per year, along with high carbohydrates content for valorisation (Ali Mandegari et al., 2017; Mussatto and van Loosdrecht, 2016).

Techno-economic analysis (TEA) is broadly used to quantify the technical and economic performance of a biorefinery based on financial return on capital investment (Brown, 2015). Simulation development is the threshold of the TEA to establish an accurate mass and energy balance of the process which is applied for estimation of equipment costing (capital cost) and operating costs (Ali Mandegari et al., 2016; Brown, 2015). Techno-economic results are usually associated with uncertainty, mainly due to the fluctuation of economic parameters (Wang et al., 2015). Therefore, techno-economic results can be supplemented by sensitivity analysis and Mote Carlo simulation. The former is applied to unearth the effect of different involved parameters and finding the predominant ones while the latter is used to calculate the probability distribution of the results considering the variation of the effective parameters (Awudu and Zhang, 2012; Wang et al., 2015).

Life cycle Assessment (LCA) is a cradle-to-grave approach formalized by the International Organization for Standardization (ISO, 2006), which is regarded as a valuable environmental screening and assessment tool with increasing application to chemical industries. The life cycle methodology was followed to investigate BD production from first generation bioethanol in a previous study (Cespi et al., 2016).

The aim of the present study is to investigate bioethanol-based BD production from a life cycle perspective in conjunction with techno-economic assessment, sensitivity analysis and Monte Carlo simulation on product selling price, whereas bioethanol production from sugarcane bagasse and harvesting residue (brown leaves) in a biorefinery annexed to a typical sugar mill is considered to simulate representative industrial conditions. To the knowledge of the authors, exploitation of sugarcane lignocellulose residues from sugar mills, as a renewable feedstock for production of BD, has not been investigated with such a comprehensive simulations incorporating economic and environmental assessments. The further evaluation of economic results were followed by sensitivity analysis and Monte Carlo simulation to determine the uncertainty and risk on the techno-economic findings.

2. Materials and methods

Four biorefinery scenarios were developed for production of ethanol or butadiene with co-production of electricity, in the context where each would be annexed to an existing sugar mill. Two different approaches were assessed for providing the energy requirement of biorefinery and sugar mill by the combined heat and power (CHP) unit; (1) energy self-sufficient scenarios where a portion of feedstock was burnt in the CHP unit, (2) coal burning scenarios where the limited energy available in biomass residues was supplemented by co-combustion of coal in the CHP unit. All of the process scenarios required installation of a new, high-efficiency CHP system to provide the process energy requirements of the sugar mill and associated biorefinery. Based on previous estimations for a typical sugar mill with a crushing capacity of 300 tonnes per hour (t/h) cane, the total lignocellulose and harvesting residues available for the biorefinery was assumed at 45 t/h dry matter (DM) bagasse and 20 t/h DM trash (brown leaves) with moisture contents of 50 wt.% and 15 wt.%, respectively (Petersen et al., 2015). The mean mass composition of bagasse and trash mixture was assumed to be 40.7% cellulose, 27.1% hemicellulose, 21.9% lignin, 3.5% ash and 6.7% extractives (Ali Mandegari et al., 2017; Petersen et al., 2015). The energy demand of an efficient sugar mill was assumed to be 0.4 tonne steam and 36.7 kWh electricity per tonne of crushed cane (Farzad et al., 2017).